



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2022 – 12:05 AM JST

PDB ID : 7VUK
Title : Crystal Structure of the core region of Thermus thermophilus MutS2 complexed with ADP.
Authors : Fukui, K.; Yano, T.
Deposited on : 2021-11-02
Resolution : 3.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

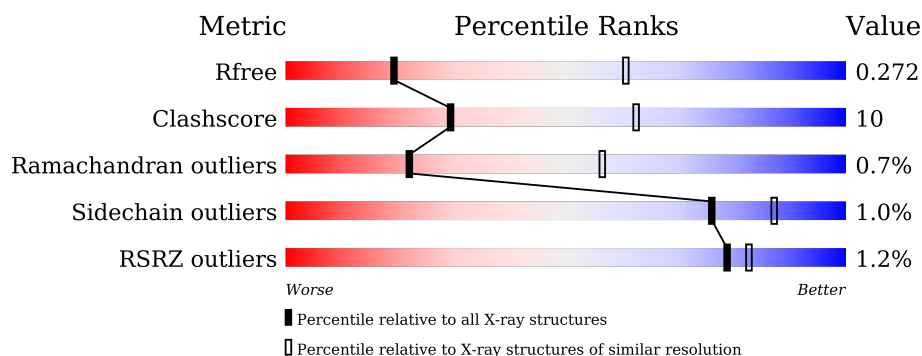
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	488	<div> <div>2%</div> <div>62%</div> <div>21%</div> <div>•</div> <div>14%</div> </div>
1	B	488	<div> <div>74%</div> <div>22%</div> <div>••</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6596 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Endonuclease MutS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			2952	1879	505	561	7			
1	B	472	Total	C	N	O	S	0	0	0
			3445	2194	600	643	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Na	0	0
			5	5		
3	B	3	Total	Na	0	0
			3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

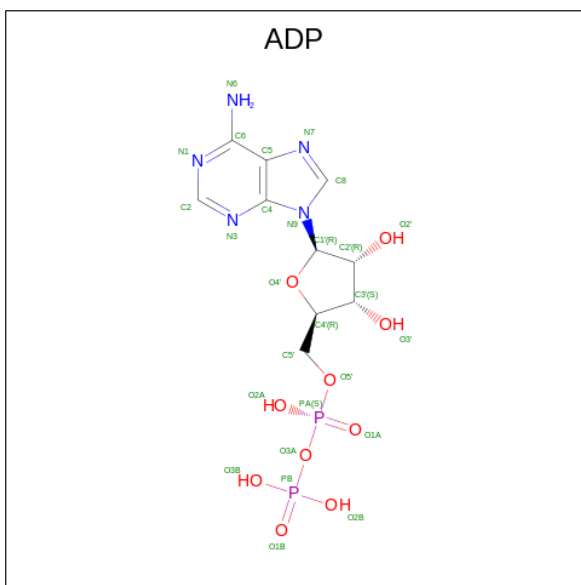
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
6	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

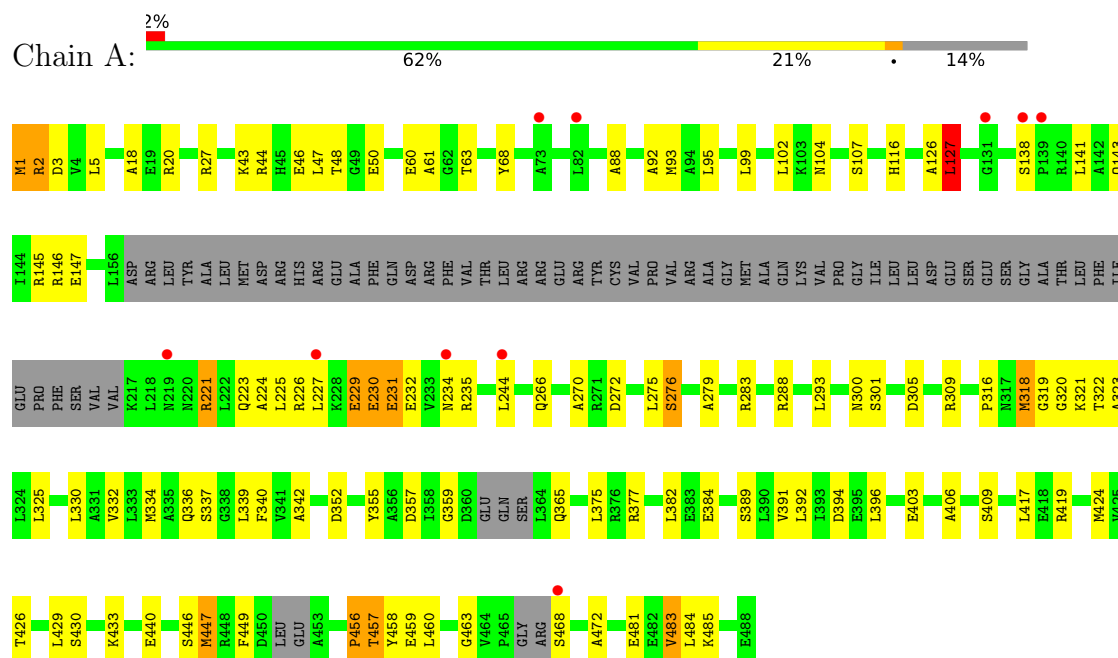
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	26	Total O 26 26	0	0
7	B	33	Total O 33 33	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Endonuclease MutS2



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.65Å 133.65Å 197.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 3.38 49.37 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.37-3.38) 99.9 (49.37-3.38)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.267 , 0.272 0.268 , 0.272	Depositor DCC
R_{free} test set	1269 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6596	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NA, ADP, CL, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/2994	0.51	0/4084
1	B	0.26	0/3495	0.50	0/4745
All	All	0.26	0/6489	0.51	0/8829

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	25
1	B	0	30
All	All	0	55

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
1	A	127	LEU	Peptide
1	A	146	ARG	Peptide
1	A	2	ARG	Peptide
1	A	221	ARG	Peptide
1	A	229	GLU	Peptide
1	A	230	GLU	Peptide
1	A	231	GLU	Peptide
1	A	232	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	234	ASN	Peptide
1	A	276	SER	Peptide
1	A	318	MET	Peptide
1	A	323	ALA	Peptide
1	A	359	GLY	Peptide
1	A	365	GLN	Peptide
1	A	440	GLU	Peptide
1	A	446	SER	Peptide
1	A	456	PRO	Peptide
1	A	457	THR	Peptide
1	A	463	GLY	Peptide
1	A	468	SER	Peptide
1	A	472	ALA	Peptide
1	A	483	VAL	Peptide
1	A	484	LEU	Peptide
1	A	61	ALA	Peptide
1	B	1	MET	Peptide
1	B	136	GLU	Peptide
1	B	153	GLN	Peptide
1	B	154	GLN	Peptide
1	B	155	ILE	Peptide
1	B	156	LEU	Peptide
1	B	157	ASP	Peptide
1	B	160	TYR	Peptide
1	B	162	LEU	Peptide
1	B	163	MET	Peptide
1	B	172	ASP	Peptide
1	B	173	ARG	Peptide
1	B	189	GLY	Peptide
1	B	192	GLN	Peptide
1	B	193	LYS	Peptide
1	B	208	LEU	Peptide
1	B	209	PHE	Peptide
1	B	221	ARG	Peptide
1	B	314	SER	Peptide
1	B	315	GLY	Peptide
1	B	341	VAL	Peptide
1	B	366	GLU	Peptide
1	B	367	ASN	Peptide
1	B	369	SER	Peptide
1	B	456	PRO	Peptide
1	B	457	THR	Peptide

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Mol	Chain	Res	Type	Group
1	B	467	ARG	Peptide
1	B	484	LEU	Peptide
1	B	60	GLU	Peptide
1	B	62	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2952	0	2780	68	0
1	B	3445	0	3386	54	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	0	0
3	B	3	0	0	0	0
4	A	2	0	0	1	0
4	B	1	0	0	0	0
5	A	42	0	60	3	0
5	B	28	0	40	1	0
6	A	27	0	12	4	0
6	B	27	0	12	1	0
7	A	26	0	0	1	0
7	B	33	0	0	0	0
All	All	6596	0	6290	122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:HD21	1:B:348:LEU:HD21	1.47	0.96
1:B:288:ARG:H	1:B:301:SER:HB3	1.44	0.82
1:A:456:PRO:HG2	1:A:458:TYR:HE1	1.43	0.81
1:A:483:VAL:HB	1:A:485:LYS:HG3	1.63	0.81
1:A:288:ARG:H	1:A:301:SER:HB3	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LYS:NZ	4:A:509:CL:CL	2.53	0.74
1:A:20:ARG:NH1	1:A:272:ASP:OD2	2.22	0.72
1:A:320:GLY:HA3	1:A:447:MET:HG2	1.72	0.71
1:B:47:LEU:HB3	1:B:263:VAL:HG11	1.74	0.70
1:A:430:SER:HA	1:A:433:LYS:HE2	1.74	0.68
1:B:297:ALA:O	1:B:299:ARG:NH1	2.28	0.67
1:A:456:PRO:HG2	1:A:458:TYR:CE1	2.29	0.65
1:A:316:PRO:HG2	1:A:449:PHE:CE1	2.32	0.64
1:A:309:ARG:NH1	1:A:417:LEU:O	2.32	0.63
1:A:270:ALA:HA	1:A:275:LEU:HB2	1.81	0.62
1:A:300:ASN:HD21	1:A:459:GLU:HA	1.64	0.62
1:A:283:ARG:HD2	1:A:305:ASP:HB3	1.81	0.62
1:A:275:LEU:HB3	1:A:340:PHE:HB3	1.81	0.61
1:A:394:ASP:OD1	1:A:426:THR:OG1	2.15	0.61
1:A:293:LEU:HD13	5:A:513:PEG:H41	1.83	0.60
1:B:280:PHE:HA	1:B:348:LEU:O	2.02	0.60
1:B:313:ILE:HB	1:B:426:THR:HG22	1.84	0.60
1:A:355:TYR:OH	1:A:384:GLU:O	2.15	0.59
1:B:316:PRO:HG3	1:B:469:TYR:CE2	2.38	0.59
1:A:449:PHE:CZ	1:A:456:PRO:HB3	2.38	0.59
1:B:450:ASP:O	1:B:454:LEU:N	2.36	0.58
1:B:457:THR:HB	1:B:459:GLU:H	1.68	0.57
1:B:25:LEU:HD12	1:B:61:ALA:HB1	1.87	0.57
1:A:457:THR:OG1	1:A:459:GLU:N	2.34	0.57
1:A:1:MET:HB3	1:A:3:ASP:H	1.70	0.57
1:A:279:ALA:HB1	5:A:514:PEG:H32	1.87	0.55
1:B:66:GLU:OE1	5:B:510:PEG:O1	2.21	0.55
1:A:88:ALA:O	1:A:92:ALA:N	2.39	0.54
1:B:449:PHE:CZ	1:B:456:PRO:HB3	2.42	0.54
1:A:403:GLU:CG	5:A:515:PEG:H12	2.37	0.54
1:B:24:PRO:HA	1:B:27:ARG:HB3	1.88	0.54
1:B:25:LEU:HD21	1:B:65:ARG:HD3	1.90	0.53
1:B:352:ASP:N	1:B:352:ASP:OD1	2.40	0.53
1:B:480:PRO:HB2	1:B:483:VAL:HG23	1.91	0.53
1:B:324:LEU:HD12	1:B:447:MET:CE	2.40	0.52
1:A:221:ARG:HD2	1:A:224:ALA:HB3	1.92	0.52
1:B:375:LEU:HD21	1:B:408:LEU:HD21	1.92	0.52
1:A:382:LEU:O	1:A:419:ARG:NH2	2.37	0.52
1:B:324:LEU:HD12	1:B:447:MET:HE1	1.92	0.52
1:A:95:LEU:O	1:A:99:LEU:N	2.40	0.51
1:A:320:GLY:N	6:A:517:ADP:O2A	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:HD12	1:B:131:GLY:HA2	1.92	0.51
1:B:96:LYS:HD2	1:B:113:ILE:HB	1.92	0.51
1:A:449:PHE:CE1	1:A:456:PRO:HB3	2.46	0.50
1:B:123:VAL:HG13	1:B:127:LEU:HD21	1.93	0.50
1:B:99:LEU:O	1:B:107:SER:OG	2.25	0.50
1:B:286:LEU:HD12	1:B:302:PHE:CZ	2.47	0.50
1:A:138:SER:HG	1:A:141:LEU:H	1.53	0.50
1:B:20:ARG:NH1	1:B:272:ASP:OD2	2.44	0.50
1:B:23:THR:HG21	1:B:61:ALA:HB3	1.93	0.50
1:A:143:GLN:O	1:A:145:ARG:N	2.38	0.50
1:B:332:VAL:HG22	1:B:348:LEU:HD13	1.94	0.50
1:A:325:LEU:CD2	1:A:424:MET:HG2	2.42	0.49
1:B:80:PRO:HA	1:B:83:LEU:HB3	1.95	0.49
1:A:319:GLY:HA3	6:A:517:ADP:O3B	2.12	0.49
1:B:78:SER:HB3	1:B:81:GLU:HB2	1.96	0.48
1:B:294:ILE:HG21	6:B:511:ADP:C2	2.49	0.48
1:B:309:ARG:HH21	1:B:441:GLY:HA3	1.77	0.48
1:B:456:PRO:HG2	1:B:458:TYR:HE1	1.78	0.48
1:B:335:ALA:HB2	1:B:341:VAL:HG11	1.96	0.47
1:B:2:ARG:HG3	1:B:3:ASP:H	1.80	0.47
1:A:230:GLU:HB3	1:A:231:GLU:HA	1.97	0.47
1:A:27:ARG:NH1	7:A:603:HOH:O	2.45	0.47
1:A:321:LYS:HG3	6:A:517:ADP:O1B	2.13	0.47
1:A:18:ALA:HB1	1:A:27:ARG:HG3	1.96	0.47
1:B:334:MET:HB3	1:B:339:LEU:HB2	1.97	0.47
1:A:2:ARG:HA	1:A:5:LEU:H	1.80	0.47
1:B:456:PRO:HB2	1:B:458:TYR:CD1	2.50	0.47
1:A:102:LEU:HD12	1:A:102:LEU:H	1.80	0.47
1:B:368:LEU:HA	1:B:371:PHE:HB3	1.97	0.46
1:A:126:ALA:HB3	1:A:127:LEU:HD23	1.98	0.46
1:A:93:MET:HE1	1:A:116:HIS:HB2	1.97	0.46
1:B:484:LEU:N	1:B:485:LYS:HB2	2.30	0.46
1:B:286:LEU:HD21	1:B:348:LEU:CD2	2.31	0.46
1:A:456:PRO:HB2	1:A:458:TYR:HD1	1.81	0.46
1:B:72:LEU:HD23	1:B:245:ALA:HB1	1.98	0.46
1:A:68:TYR:HD1	1:A:244:LEU:HG	1.82	0.45
1:A:43:LYS:O	1:A:46:GLU:N	2.50	0.45
1:A:357:ASP:OD1	1:A:377:ARG:HD2	2.18	0.44
1:A:330:LEU:O	1:A:334:MET:HB2	2.16	0.44
1:A:221:ARG:NH1	1:A:225:LEU:H	2.15	0.44
1:B:309:ARG:NH1	1:B:417:LEU:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:O	1:A:336:GLN:HG3	2.19	0.43
1:A:48:THR:HB	1:A:340:PHE:HE1	1.83	0.43
1:A:266:GLN:HG2	1:A:339:LEU:HD21	2.01	0.43
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.91	0.43
1:B:159:LEU:H	1:B:159:LEU:HD23	1.83	0.43
1:A:300:ASN:OD1	1:A:460:LEU:N	2.32	0.43
1:A:322:THR:HG23	1:A:394:ASP:OD2	2.19	0.43
1:B:62:GLY:HA2	1:B:65:ARG:HB3	2.00	0.43
1:B:107:SER:O	1:B:111:GLU:HG3	2.19	0.43
1:A:406:ALA:HA	1:A:429:LEU:HD23	1.99	0.43
1:B:133:VAL:HG21	1:B:233:VAL:HG13	2.00	0.43
1:B:218:LEU:H	1:B:218:LEU:HD23	1.83	0.43
1:A:223:GLN:O	1:A:227:LEU:N	2.32	0.43
1:A:276:SER:OG	1:A:276:SER:O	2.37	0.43
1:B:194:VAL:O	1:B:211:GLU:HB3	2.19	0.43
1:A:318:MET:N	6:A:517:ADP:O3B	2.39	0.42
1:A:352:ASP:OD1	1:A:352:ASP:N	2.50	0.42
1:A:50:GLU:OE1	1:A:104:ASN:HB2	2.20	0.41
1:B:289:ALA:N	1:B:300:ASN:O	2.39	0.41
1:A:391:VAL:O	1:A:392:LEU:HD23	2.19	0.41
1:B:357:ASP:HA	1:B:377:ARG:HD2	2.03	0.41
1:A:396:LEU:HG	1:A:409:SER:HB3	2.02	0.41
1:B:270:ALA:HA	1:B:275:LEU:HB2	2.01	0.41
1:A:481:GLU:CB	1:A:483:VAL:HG22	2.51	0.41
1:A:325:LEU:HD23	1:A:424:MET:HG2	2.01	0.41
1:B:355:TYR:OH	1:B:384:GLU:O	2.26	0.41
1:A:223:GLN:O	1:A:226:ARG:N	2.54	0.41
1:B:310:ILE:HA	1:B:423:GLY:O	2.21	0.41
1:A:275:LEU:HD23	1:A:342:ALA:HA	2.02	0.40
1:A:99:LEU:O	1:A:107:SER:OG	2.27	0.40
1:B:120:LEU:O	1:B:124:ARG:HG2	2.21	0.40
1:B:288:ARG:NH2	1:B:299:ARG:HD3	2.37	0.40
1:A:457:THR:HG1	1:A:459:GLU:H	1.65	0.40
1:A:44:ARG:HA	1:A:47:LEU:HD13	2.04	0.40
1:A:60:GLU:HB3	1:A:63:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/488 (84%)	373 (91%)	35 (8%)	3 (1%)	22	56
1	B	464/488 (95%)	438 (94%)	23 (5%)	3 (1%)	25	59
All	All	875/976 (90%)	811 (93%)	58 (7%)	6 (1%)	22	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ARG
1	B	158	ARG
1	B	193	LYS
1	A	147	GLU
1	A	229	GLU
1	B	157	ASP

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/392 (66%)	253 (98%)	4 (2%)	62	81
1	B	320/392 (82%)	318 (99%)	2 (1%)	86	93
All	All	577/784 (74%)	571 (99%)	6 (1%)	76	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LEU
1	A	337	SER
1	A	389	SER
1	A	447	MET
1	B	213	PHE
1	B	231	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	428	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 16 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ADP	B	511	2	24,29,29	0.92	1 (4%)	29,45,45	1.44	4 (13%)
5	PEG	A	516	-	6,6,6	0.10	0	5,5,5	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	A	513	-	6,6,6	0.14	0	5,5,5	0.04	0
5	PEG	B	510	-	6,6,6	0.10	0	5,5,5	0.10	0
6	ADP	A	517	2	24,29,29	1.00	1 (4%)	29,45,45	1.49	4 (13%)
5	PEG	A	514	-	6,6,6	0.13	0	5,5,5	0.06	0
5	PEG	A	515	-	6,6,6	0.27	0	5,5,5	0.61	0
5	PEG	A	511	-	6,6,6	0.12	0	5,5,5	0.07	0
5	PEG	B	509	-	6,6,6	0.13	0	5,5,5	0.08	0
5	PEG	A	512	-	6,6,6	0.14	0	5,5,5	0.07	0
5	PEG	B	507	-	6,6,6	0.13	0	5,5,5	0.06	0
5	PEG	B	508	-	6,6,6	0.12	0	5,5,5	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	B	511	2	-	6/12/32/32	0/3/3/3
5	PEG	A	516	-	-	4/4/4/4	-
5	PEG	A	513	-	-	2/4/4/4	-
5	PEG	B	510	-	-	1/4/4/4	-
6	ADP	A	517	2	-	2/12/32/32	0/3/3/3
5	PEG	A	514	-	-	2/4/4/4	-
5	PEG	A	515	-	-	3/4/4/4	-
5	PEG	A	511	-	-	0/4/4/4	-
5	PEG	B	509	-	-	1/4/4/4	-
5	PEG	A	512	-	-	1/4/4/4	-
5	PEG	B	507	-	-	3/4/4/4	-
5	PEG	B	508	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	517	ADP	C5-C4	2.57	1.47	1.40
6	B	511	ADP	C5-C4	2.34	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	511	ADP	C3'-C2'-C1'	3.96	106.94	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	517	ADP	C3'-C2'-C1'	3.64	106.45	100.98
6	A	517	ADP	PA-O3A-PB	-3.44	121.02	132.83
6	A	517	ADP	N3-C2-N1	-3.20	123.68	128.68
6	B	511	ADP	PA-O3A-PB	-3.11	122.16	132.83
6	B	511	ADP	N3-C2-N1	-2.74	124.39	128.68
6	A	517	ADP	C4-C5-N7	-2.65	106.64	109.40
6	B	511	ADP	C4-C5-N7	-2.46	106.84	109.40

There are no chirality outliers.

All (28) torsion outliers are listed below:

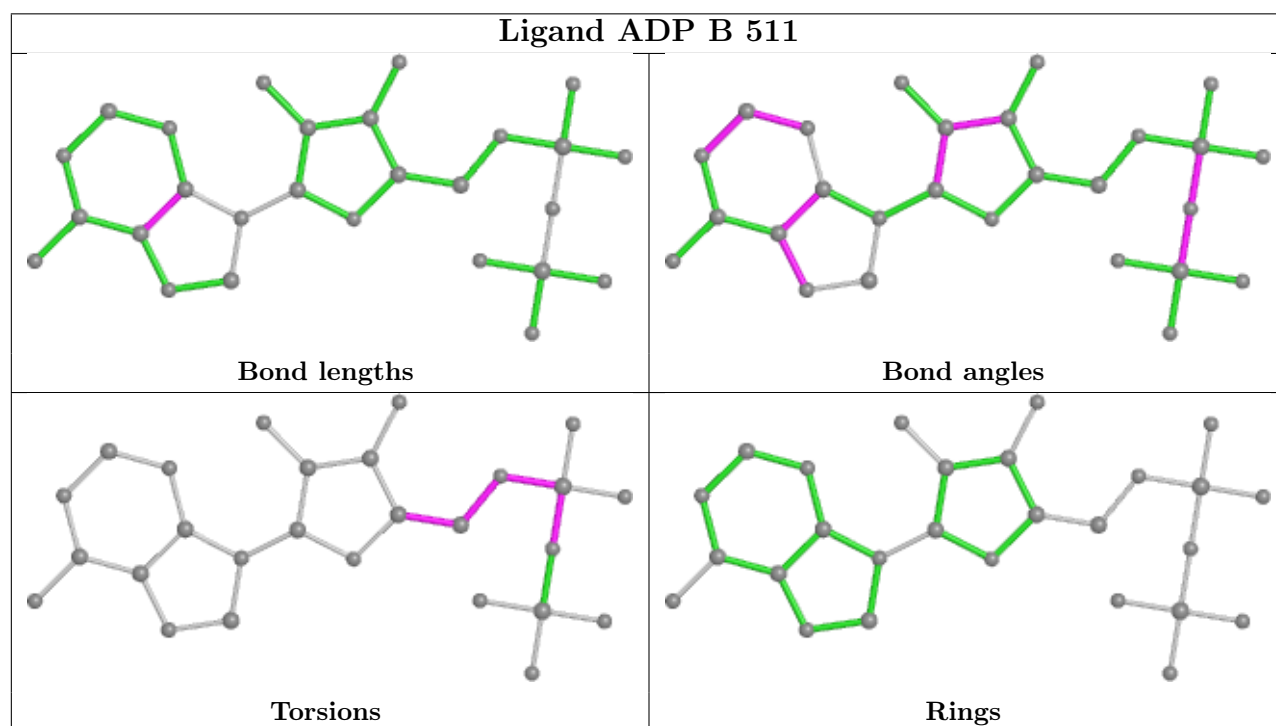
Mol	Chain	Res	Type	Atoms
6	A	517	ADP	C5'-O5'-PA-O2A
6	A	517	ADP	C5'-O5'-PA-O3A
6	B	511	ADP	C5'-O5'-PA-O2A
6	B	511	ADP	C5'-O5'-PA-O3A
5	A	516	PEG	O1-C1-C2-O2
5	A	515	PEG	O2-C3-C4-O4
5	A	513	PEG	O1-C1-C2-O2
5	B	509	PEG	O1-C1-C2-O2
5	A	516	PEG	O2-C3-C4-O4
5	A	515	PEG	C1-C2-O2-C3
5	A	512	PEG	C1-C2-O2-C3
5	B	508	PEG	C1-C2-O2-C3
5	B	508	PEG	O1-C1-C2-O2
5	A	516	PEG	C1-C2-O2-C3
5	A	513	PEG	C4-C3-O2-C2
5	B	507	PEG	C1-C2-O2-C3
5	B	507	PEG	O2-C3-C4-O4
5	A	514	PEG	C1-C2-O2-C3
5	A	516	PEG	C4-C3-O2-C2
6	B	511	ADP	C4'-C5'-O5'-PA
6	B	511	ADP	PB-O3A-PA-O2A
5	A	515	PEG	C4-C3-O2-C2
5	B	507	PEG	C4-C3-O2-C2
5	A	514	PEG	C4-C3-O2-C2
5	B	510	PEG	O1-C1-C2-O2
6	B	511	ADP	C3'-C4'-C5'-O5'
6	B	511	ADP	PB-O3A-PA-O1A
5	B	508	PEG	C4-C3-O2-C2

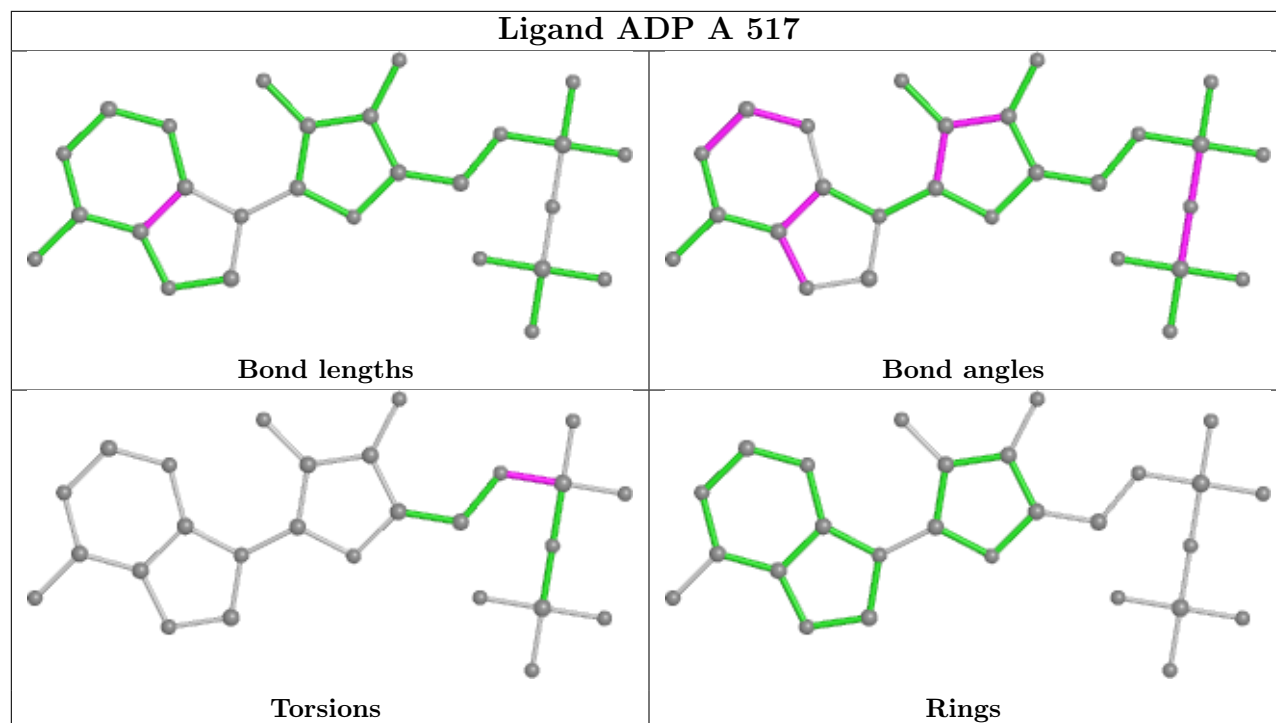
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	511	ADP	1	0
5	A	513	PEG	1	0
5	B	510	PEG	1	0
6	A	517	ADP	4	0
5	A	514	PEG	1	0
5	A	515	PEG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/488 (86%)	0.12	10 (2%) 59 62	36, 70, 144, 200	0
1	B	472/488 (96%)	-0.15	1 (0%) 95 97	37, 62, 92, 129	0
All	All	893/976 (91%)	-0.02	11 (1%) 79 83	36, 65, 124, 200	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	GLY	3.5
1	A	82	LEU	2.8
1	A	468	SER	2.7
1	A	219	ASN	2.6
1	A	73	ALA	2.5
1	A	138	SER	2.4
1	A	139	PRO	2.4
1	A	227	LEU	2.4
1	B	212	PRO	2.3
1	A	244	LEU	2.2
1	A	234	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

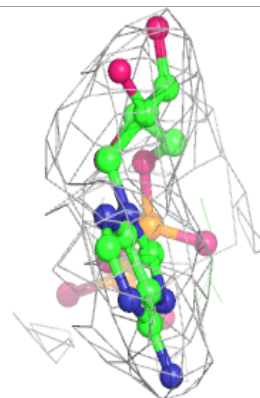
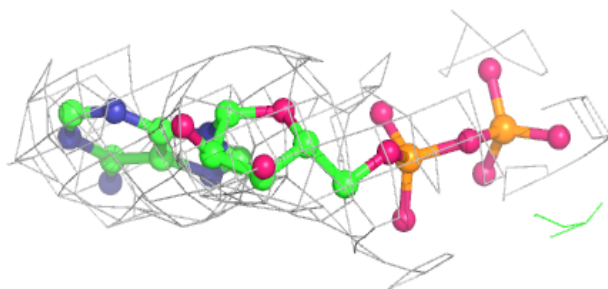
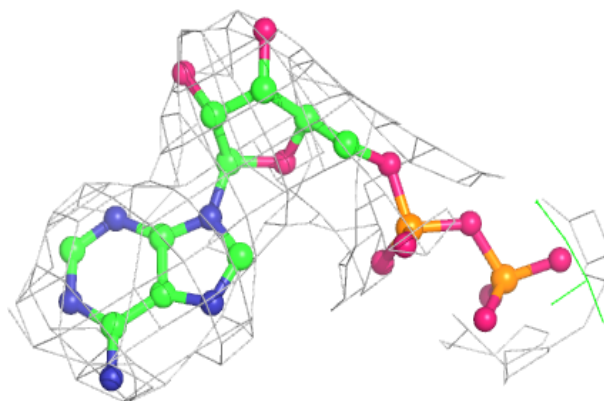
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	503	1/1	0.76	0.19	46,46,46,46	0
5	PEG	A	515	7/7	0.77	0.34	74,79,87,88	0
5	PEG	A	513	7/7	0.79	0.23	49,69,79,87	0
3	NA	A	505	1/1	0.79	0.15	37,37,37,37	0
5	PEG	B	507	7/7	0.80	0.33	56,61,74,79	0
5	PEG	B	509	7/7	0.80	0.33	43,61,77,82	0
3	NA	A	506	1/1	0.81	0.19	26,26,26,26	0
5	PEG	B	508	7/7	0.83	0.40	54,57,73,82	0
5	PEG	B	510	7/7	0.84	0.43	71,74,78,83	0
5	PEG	A	514	7/7	0.86	0.37	58,64,71,88	0
5	PEG	A	511	7/7	0.87	0.29	63,66,67,67	0
3	NA	B	504	1/1	0.88	0.80	57,57,57,57	0
5	PEG	A	516	7/7	0.90	0.42	64,72,93,95	0
3	NA	B	505	1/1	0.91	0.21	25,25,25,25	0
5	PEG	A	512	7/7	0.92	0.27	36,48,53,69	0
4	CL	B	506	1/1	0.92	0.20	63,63,63,63	0
3	NA	A	504	1/1	0.92	0.20	38,38,38,38	0
4	CL	A	510	1/1	0.93	0.15	54,54,54,54	0
4	CL	A	509	1/1	0.93	0.14	76,76,76,76	0
2	MG	A	501	1/1	0.94	0.49	45,45,45,45	0
3	NA	A	508	1/1	0.94	0.31	32,32,32,32	0
3	NA	B	503	1/1	0.94	0.18	33,33,33,33	0
3	NA	A	507	1/1	0.95	0.37	31,31,31,31	0
2	MG	B	502	1/1	0.95	0.22	42,42,42,42	0
6	ADP	A	517	27/27	0.95	0.19	45,61,66,67	0
6	ADP	B	511	27/27	0.95	0.17	48,54,62,66	0
2	MG	A	502	1/1	0.96	0.15	33,33,33,33	0
2	MG	B	501	1/1	0.98	0.31	35,35,35,35	0

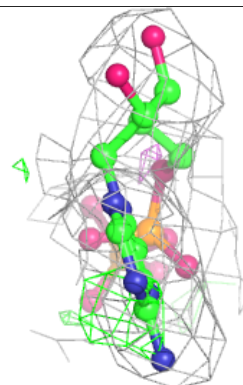
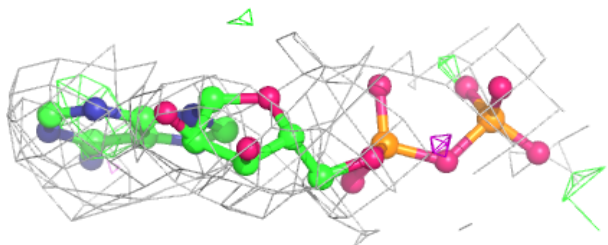
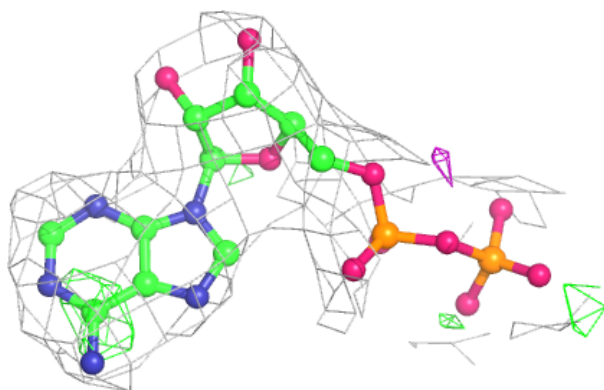
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 517:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP B 511:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.